Schwinger-Keldysh Semionic Approach for Quantum Spin Systems

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We derive a path-integral Schwinger-Keldysh approach for quantum spin systems. This is achieved by means of a semionic representation of spins as fermions with imaginary chemical potential. The major simplifying feature in comparison with other representations (Holstein-Primakoff, Dyson-Maleev, slave bosons/fermions, etc.) is that the local constraint is taken into account exactly. As a result, the standard diagram technique with the usual Feynman codex is constructed. We illustrate the application of this technique for the Néel and spin-liquid states of the antiferromagnetic Heisenberg model.

For a long time [1] physicists have been aware of the fact that spin operators which commute on different sites and anticommute on the same site are neither Fermi nor Bose operators. Less convergent opinions exist on whether fermionizations or bosonizations or none of those should be used to take care of spin statistics in many body quantum theory. At least the answers appear to be linked to the type of physical problem considered. The widely accepted view is that path integral representations and diagrammatic expansions for spin systems are thus substantially more complicated than those of pure fermion/boson systems. Many variants of the diagram technique [2], which are based on different representation of spins such as Bose [1–4], Fermi [5–7], Majorana [8], supersymmetric [9], or Hubbard [10] operators, have been proposed. Another method to treat spin Hamiltonians is based on direct representation of coherent states for spins (nonlinear σ model, see, e.g., [8]). Some of these techniques [1–10], being applicable only at low temperatures or in large spin ($S \gg 1$) limit, nevertheless describe well the excitations in ordered magnets (ferromagnetic and antiferromagnetic magnons), but fail to provide rigorous calculations in strongly correlated systems such as Kondo lattices or quantum magnets. Other techniques, based on a successful choice for the hierarchy of coupling constants, are mainly restricted to equilibrium situations. The fundamental problem which is at the heart of the difficulty is the local constraint. On one hand, any representation of spin operators as a bilinear combination of Fermi or Bose quasiparticles makes the dimensionality of the Hilbert space, where these operators act, greater than the dimensionality of the Hilbert space for spin operators. As a result, the spurious unphysical states should be excluded from the consideration, resulting in substantial complication of corresponding rules of diagrammatical summation. On the other hand, there is no Wick theorem directly for spin operators but the Gaudin theorem [11] instead (see also [7,10]). It cannot, however, avoid complications in diagram techniques based on Hubbard operators, rendering the resummation of diagram series in many cases practically uncontrollable. The exclusion of double-occupied and empty states for impurity spins interacting with a conduction electron bath (single

impurity Kondo problem) [6] is cured by an infinite chemical potential for Abrikosov pseudofermions. It works for dilute spin subsystems, where all spins can be considered independently. Unfortunately, attempts to generalize this technique to the lattice of spins result in the replacement of the local constraint (the number of particles on each site is fixed) by a so-called global constraint (in the saddle point approximation), where the number of particles is fixed only as an average value for the whole crystal. There is no reason to believe that such an approximation is a good starting point for the description of strongly correlated systems. Besides, it is very difficult to take into account the fluctuations related to the replacement of a local constraint by a global one.

An alternative approach for spin Hamiltonians free of the local constraint problem has been proposed in the pioneering paper of Popov and Fedotov (PF) [12]. Based on the exact fermionic representation for $S = 1/2$ and $S = 1$ operators, where fermions are treated as quasiparticles with imaginary chemical potential, these authors demonstrated the power and simplification of the corresponding Matsubara diagram technique. For these two special cases the Matsubara frequencies are $\omega_n = 2\pi T(n + 1/4)$ for $S = 1/2$ and $\omega_n = 2\pi T(n + 1/3)$ for $S = 1$, providing a rigorous description of (and restricted to) the equilibrium situation. The semionic representation used by PF is neither fermionic nor bosonic, but reflects the fundamental Pauli nature of spins. Later, the generalization of the PF technique for arbitrary spin [13] was derived by introducing proper chemical potentials for spin fermions. The goal of this paper is to derive a method for nonequilibrium systems, which allows one to treat quantum spin Hamiltonians on the same footing as Fermi or Bose systems.

A long time ago Keldysh [14] proposed a novel approach for the description of kinetic phenomena in metals. This approach was found especially fruitful for normal metals [15], and, in many recent applications, for superconductors [16] and for disordered interacting (normal or superconducting) electron liquids [17], for example. The previous application of the real-time formalism to the quantum theory of Bose-Einstein condensation (BEC) [18] allowed the derivation of a Fokker-Planck equation,

which describes both kinetic and coherent stages of BEC. Moreover, Ref. [19] developed the closed-time path integral formalism for aging effects in quantum disordered systems being in contact with an environment. The Keldysh formalism in application to disordered systems (see [20,21]) also attracted interest some time ago as an alternative approach to the replica technique. The main advantage of closed-time contour calculations is an automatic normalization (disorder independent) of the partition function. In this paper we derive the Keldysh formalism for quantum spin systems (e.g., Heisenberg clean and disordered magnets, Kondo systems [22,23]), which is based on PF ideas of semionic representation.

We reformulate the PF concept by adopting it to real-time formalism. As an example, we consider $S = 1/2$. As it was first shown in [12] (see also [24]), the partition function of a spin system with Hamiltonian H_S can be replaced by the partition function of an effective "fermionic" system with Hamiltonian H_F as follows

$$Z_S = \mathrm{Tr}\, e^{-\beta \hat{H}_S} = (\pm i)^N \, \mathrm{Tr}\, e^{-\beta(\hat{H}_F \pm i\pi \hat{N}_F/2\beta)}, \quad (1)$$

where $\beta = 1/T$, and the usual fermionic representation of spin similar to, e.g., Abrikosov pseudofermions [6] is used: $S^+ = f_\uparrow^\dagger f_\downarrow$, $S^- = f_\downarrow^\dagger f_\uparrow$, $S^z = \frac{1}{2}(f_\uparrow^\dagger f_\uparrow - f_\downarrow^\dagger f_\downarrow)$, and $N_F = f_\uparrow^\dagger f_\uparrow + f_\downarrow^\dagger f_\downarrow$.

Representing spins as bilinear combinations of Fermi operators, we enlarged by a factor of 2 the Hilbert space of the Hamiltonian. In addition to physical states $|1,0\rangle$ and $|0,1\rangle$ two unphysical states $|1,1\rangle$ and $|0,0\rangle$ are introduced. Nevertheless, in the average over all states, unphysical states cancel each other, since $\mathrm{Tr}_{\mathrm{unphys}}[\exp(\mp i\pi/2)]^{N_F} = (\mp i)^0 + (\mp i)^2 = 0$. This representation being of semionic origin results in the conventional Matsubara diagram technique with $\omega_n = 2\pi T(n + 1/4)$ or $\omega_n = 2\pi T(n + 3/4)$, depending on the sign in expressions (1). Besides, one can introduce the auxiliary distribution function for quasiparticles [25],

$$f^{(1/2)}(\epsilon) = T\sum_n \frac{e^{i\omega_n \tau|_{+0}}}{i\omega_n - \epsilon} = \frac{1}{e^{\pm i\pi/2}\exp(\beta\epsilon) + 1}, \quad (2)$$

where $(\pm)$ signs in the exponent (2) are the same as in (1). We note that, since auxiliary Fermi fields do not represent the true quasiparticles of the problem, helping only to treat properly the spin operators, the distribution function for these objects in general should not be a real function, e.g., $f^{(1/2)} = n(2\epsilon) \mp \frac{i}{2}\mathrm{sech}(\epsilon/T)$, where $n(x) = [\exp(x/T) + 1]^{-1}$ is the standard Fermi distribution function. As we shall see for $S = 1/2$ and $S = 1$, $1 - 2\,\mathrm{Re}f^{(S)}(\epsilon) = B_S(\epsilon/T)$ is expressed in terms of the Brillouin function $B_S(x) = (1 + \frac{1}{2S}) \times \coth[(1 + \frac{1}{2S})x] - \frac{1}{2S}\coth(\frac{x}{2S})$, e.g., for $S = 1/2$, $B_{1/2}(x) = \tanh(x)$. We also note that in the $T \to 0$ limit the imaginary part of $f^{(1/2)}$ satisfies the identity $\mathrm{Im}f^{(1/2)}(x) = \mp i\pi T\delta(x)/2$.

The spin correlation functions of any order can be expressed in terms of the two-component field $\psi^T = (f_\uparrow f_\downarrow)$:

$$\langle S_{i_1}^{\alpha_1}(t_1)\cdots S_{i_n}^{\alpha_n}(t_n)\rangle = \mathrm{Tr}[\rho_0(\psi^\dagger \sigma_{i_1}^{\alpha_1}\psi)_{t_1}\cdots(\psi^\dagger \sigma_{i_n}^{\alpha_n}\psi)_{t_n}],$$

where $\rho_0 = \exp(-\beta H_0)/\mathrm{Tr}\exp(-\beta H_0)$ is the density matrix and σ denotes Pauli matrices. We included the term $i\pi N_F/(2\beta)$ into the Hamiltonian $H_0 = -h\sum_i S_i^z \pm i\pi T/2\sum_i N_F^{(i)}$ of noninteracting spins in a uniform external magnetic field h, since it exists both in the numerator and denominator of ρ_0.

Following the standard route [26] we can express the partition function of the problem containing spin operators as a path integral over Grassmann variables $\bar\psi, \psi$

$$Z/Z_0 = \int D\bar\psi D\psi \exp(i\mathcal{A}) \Big/ \int D\bar\psi D\psi \exp(i\mathcal{A}_0), \quad (3)$$

where actions $\mathcal{A}$ and $\mathcal{A}_0$ are taken as an integral along the closed-time contour $C_t + C_\tau$ which is shown in Fig. 1. The contour is closed at $t = -\infty + i\tau$ since $\exp(-\beta H_0) = T_\tau \exp(-\int_0^\beta H_0\,d\tau)$. We denote the ψ fields on the upper and lower sides of the contour C_t as ψ_1 and ψ_2, respectively. The fields Ψ stand for the contour C_τ. These fields provide matching conditions for $\psi_{1,2}$ and are excluded from final expressions. Taking into account the semionic boundary conditions for generalized Grassmann fields $\Psi^\mu(\beta) = i\Psi^\mu(0)$, $\bar\Psi^\mu(\beta) = -i\bar\Psi^\mu(0)$, one gets the matching conditions for $\psi_{1,2}$ at $t = \pm\infty$,

$$\psi_1^\mu(-\infty) = i\psi_2^\mu(-\infty), \qquad \psi_1^\mu(+\infty) = \psi_2^\mu(+\infty). \quad (4)$$

The correlation functions can be represented as a functional derivation of the generating functional

$$Z[\eta] = Z_0^{-1}\int D\bar\psi D\psi$$

$$\times \exp\left(i\mathcal{A} + i\oint_C dt\,(\bar\eta\sigma^z\psi + \bar\psi\sigma^z\eta)\right),$$

where η represents sources and the σ^z matrix stands for "causal" and "anticausal" orderings along the contour.

The on-site Green's functions (GF's) which are matrices 4×4 with respect to both Keldysh (lower) and spin (upper) indices are given by

$$G_{\mu\nu}^{\alpha\beta}(t,t') = -i\frac{\delta}{i\delta\bar\eta_\mu^\alpha(t)}\frac{\delta}{i\delta\eta_\nu^\beta(t')}Z[\eta]\big|_{\bar\eta,\eta\to 0}.$$

After a standard shift transformation [26] of fields ψ the Keldysh GF of free PF fermions assumes the form
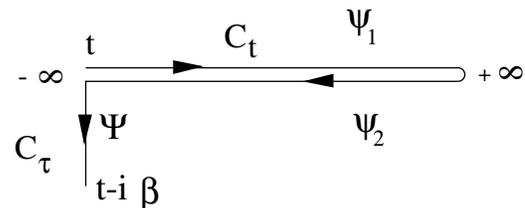
FIG. 1. Keldysh double side contour going along real-time axis $-\infty \to +\infty \to -\infty$ and "closed" in imaginary time.

$$G_0^\alpha(\epsilon) = G_0^{R,\alpha}\begin{pmatrix} 1 - f_\epsilon & -f_\epsilon \\ 1 - f_\epsilon & -f_\epsilon \end{pmatrix}$$
$$- G_0^{A,\alpha}\begin{pmatrix} -f_\epsilon & -f_\epsilon \\ 1 - f_\epsilon & 1 - f_\epsilon \end{pmatrix},$$

where the retarded and advanced GF's are

$$G_0^{(R,A)\alpha}(\epsilon) = (\epsilon + \sigma_{\alpha\alpha}^z h/2 \pm i\delta)^{-1},$$
$$f_\epsilon = f^{(1/2)}(\epsilon). \tag{5}$$

The interdependence of matrix elements of the GF in Keldysh space is more transparent after rotation

$$\hat{G} \Rightarrow \frac{1 - i\sigma^y}{\sqrt{2}}\sigma^z G \frac{1 + i\sigma^y}{\sqrt{2}} = \begin{pmatrix} G^R & G^K \\ 0 & G^A \end{pmatrix}, \tag{6}$$

where $G_0^K = -i2\pi\delta(\epsilon \pm h/2)[B_{1/2}(\epsilon/T) \pm i\,\text{sech}(\epsilon/T)]$. We emphasize that, unlike diagrammatic techniques for Fermi and Bose operators, the off-diagonal element (Keldysh component) in semionic representation is expressed in terms of a Brillouin function, containing correct information about occupied states. We recall that diagonal elements of the matrix (6) in "triangular" representation satisfy the Dyson equation providing the exact description of the system. The equation of motion for G^K generally constitutes the quantum-kinetic equation.

Let us illustrate the application of the Schwinger-Keldysh formalism for spin Hamiltonians. We consider the Heisenberg model with nearest neighbor interaction

$$H_{\text{int}} = -\sum_{\langle ij \rangle} J_{ij}\left(\vec{S}_i\vec{S}_j - \frac{1}{4}\right) = \frac{1}{2}\sum_{\langle ij \rangle} J_{ij}\psi_i^\dagger\psi_j\psi_j^\dagger\psi_i.$$

We firstly discuss the *Néel solution* for the Heisenberg model with isotropic antiferromagnetic (AFM) exchange ($J < 0$). By applying the PF transformation to the partition function, one obtains the action as an integral along the closed-time Keldysh contour,

$$\mathcal{A} = \mathcal{A}_0 + \mathcal{A}_{\text{int}} = \mathcal{A}_0 + \oint_C dt \sum_{\mathbf{q}} J(\mathbf{q})\vec{S}_{\mathbf{q}}(t)\vec{S}_{-\mathbf{q}}(t), \tag{7}$$

where $\mathcal{A}_0$ corresponds to noninteracting PF fermions

$$\mathcal{A}_0 = \oint_C dt \sum_i \bar{\psi}_i\begin{pmatrix} (G_0^{R,\alpha})^{-1} & 0 \\ 0 & (G_0^{A,\alpha})^{-1} \end{pmatrix}\psi_i. \tag{8}$$

We denote $J_{\mathbf{q}} = J\sum_{\langle l \rangle} e^{i\mathbf{q}\mathbf{l}}$, $\nu_{\mathbf{q}} = J_{\mathbf{q}}/J_0$ and apply the eight-component PF representation with $\psi^T = (\tilde{\psi}_{\mathbf{k}}^T \tilde{\psi}_{\mathbf{k}+\mathbf{Q}}^T)$, where $\mathbf{Q} = (\pi, \ldots, \pi)$ for hypercubic lattice. To decouple the four-fermion term along the Keldysh contour with the help of the Hubbard-Stratonovich transformation we introduce the two-Keldysh-component *vector* (Bose) field $\vec{\Phi}^T = (\vec{\Phi}_1\vec{\Phi}_2)$. As a result we obtain

$$\mathcal{A}_{\text{int}} = -\text{Tr}(\vec{\Phi}_{\mathbf{q}}^T J_{\mathbf{q}}^{-1}\sigma^z\vec{\Phi}_{\mathbf{q}}) + \text{Tr}(\bar{\psi}\vec{\Phi}_\mu\vec{\sigma}\gamma^\mu\psi). \tag{9}$$

Now we integrate out ψ fields and express the effective action in terms of $\vec{\Phi}$ fields

$$\mathcal{A}_{\text{eff}} = -\text{Tr}(\vec{\Phi}_{\mathbf{q}}^T J_{\mathbf{q}}^{-1}\sigma^z\vec{\Phi}_{\mathbf{q}}) + \text{Tr}\ln(G_0^{-1} + \vec{\Phi}_\mu\vec{\sigma}\gamma^\mu),$$

where $\gamma^\mu = (\sigma^z \pm 1)/2$ acts in Keldysh space. Since in general $\vec{\Phi}$ is a time- and space-dependent fluctuating field, the partition function (3) cannot be evaluated exactly.

Nevertheless, when a magnetic instability occurs, we can represent the longitudinal component of this field as a superposition of a staggered time-independent part ("staggered condensate") and a fluctuating field

$$\Phi_\mu^z(\mathbf{q}, \omega) = \frac{1}{2}\mathcal{N}J_{\mathbf{q}}\gamma^\mu\delta_{\mathbf{q},\mathbf{Q}}\delta(\omega) + \phi_\mu^z(\mathbf{q}, \omega), \tag{10}$$

where $\mathcal{N}$ is a staggered magnetization and $\Phi_\mu^\pm(\mathbf{q}, \omega) = \phi_\mu^\pm(\mathbf{q}, \omega)$ with the matching conditions at $t = \pm\infty$,

$$\phi_1^\pm(-\infty) = \phi_2^\pm(-\infty), \qquad \phi_1^\pm(+\infty) = \phi_2^\pm(+\infty). \tag{11}$$

We expand $\text{Tr}\ln(G_0^{-1} + \vec{\phi}_\mu\vec{\sigma}\gamma^\mu)$ in accordance with

$$\text{Tr}\ln(\cdots) = \text{Tr}\ln G_0^{-1} + \sum_{n=1}^{\infty}\frac{(-1)^{n+1}}{n}(G_0\vec{\phi}_\mu\vec{\sigma}\gamma^\mu)^n. \tag{12}$$

The spectrum of the excitations (AFM magnons) can be defined as poles of the transverse GF $D_{\mathbf{x},t}^{+,-} = D(\mathbf{x}, t) = -i\langle T_C\phi_1^+(\mathbf{x}, t)\phi_1^-(0, 0)\rangle$. The procedure of the calculation of this GF is similar to that for a fermionic GF. By introducing the sources and evaluating (12), one gets

$$D_0(\omega) = D_0^R\begin{pmatrix} 1 + N_\omega & N_\omega \\ 1 + N_\omega & N_\omega \end{pmatrix}$$
$$- D_0^A\begin{pmatrix} N_\omega & N_\omega \\ 1 + N_\omega & 1 + N_\omega \end{pmatrix},$$

where the retarded and advanced magnon GF's are

$$D_0^{R,A}(\mathbf{q}, \omega) = [\omega - \omega(\mathbf{q}) \pm i\delta]^{-1},$$
$$N_\omega = [\exp(\beta\omega) - 1]^{-1}.$$

The magnon spectrum $\omega_{\mathbf{q}}$ is determined by the zeros of the expression $J_{\mathbf{q}}^{-1} - \Pi_2^{+-}(\omega)$ (see Fig. 2a) in equilibrium

$$\omega_{\mathbf{q}} = |J_0|\mathcal{N}\sqrt{1 - \nu_{\mathbf{q}}^2} \Rightarrow c|\mathbf{q}|,$$
$$\mathcal{N} = \tanh\left(\frac{J_{\mathbf{Q}}\mathcal{N}}{2T}\right). \tag{13}$$

The magnon damping is defined by four-magnon processes Π_4^{+-+-}, shown in Fig. 2b. The derivation of the kinetic equation and calculation of magnon damping is reserved here for a detailed publication. The results (13) (and similar for quantum FM) are in full agreement with the spin-wave theory (see, for example, Refs. [2] and [3,7]).

The second possibility to decouple the four-fermion term in the Heisenberg model is provided by the bilocal *scalar* bosonic field Λ_{ij} depending on two sites. By introducing new coordinates $\vec{R} = (\vec{R}_i + \vec{R}_j)/2$, $\vec{\rho} = \vec{R}_i - \vec{R}_j$
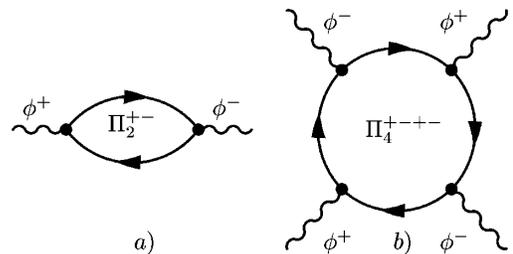
FIG. 2. Feynman diagrams contributing to dispersion (a) and damping (b) of magnons. The solid line denotes PF fermions.

and applying a Fourier transformation, we obtain the effective action

$$\mathcal{A}_{\text{eff}} = -\tfrac{1}{2}\operatorname{Tr}(\Lambda_{Pq_1}^T J_{\mathbf{q_1}-\mathbf{q_2}}^{-1}\sigma^z \Lambda_{Pq_2})$$
$$+ \operatorname{Tr}\ln(G_0^{-1} - \Lambda_\mu \gamma^\mu).$$

This effective action describes the nonequilibrium quantum spin liquid (SL). We confine ourselves to consider the uniform phase [27] of *resonant valence bonds* (RVB) in 2D antiferromagnets. It is suitable to rewrite the functional in new variables, namely, the amplitude Δ and the phase $\Theta = \vec{\rho}\vec{A}(\vec{R})$, according to formula

$$\Lambda_\mu^{\langle ij\rangle}(\vec{R},\vec{\rho}) = \Delta(\vec{\rho})J\gamma^\mu \exp[i\vec{\rho}\vec{A}_\mu(\vec{R})]. \qquad (14)$$

The exponent in (14) stands for gauge fluctuations to be taken in eikonal approximation. The spectrum of excitations in the uniform SL is defined by the zeros of $\pi_{q,\omega}^{R,\alpha\beta} = \operatorname{Tr}[\,p^\alpha p^\beta(G_{p+q}^R G_p^K + G_{p+q}^K G_p^A) + \delta_{\alpha\beta}f(J_{\mathbf{p}}\Delta)]$ in equilibrium [28] and is purely diffusive (see, e.g., [27])

$$\omega_{\mathbf{q}} = iJ\Delta|\mathbf{q}|^3, \qquad \Delta = -\sum_{\mathbf{q}}\nu(\mathbf{q})\tanh\!\left(\frac{J_{\mathbf{q}}\Delta}{T}\right). \quad (15)$$

The quantum kinetic equation for nonequilibrium spin RVB liquids can be obtained by taking into account the higher order diagrams similar to Fig. 2b with currentlike vertices and will be presented elsewhere.

We discuss finally the Schwinger-Keldysh formalism for spins $S > 1/2$. As shown by Popov and Fedotov for $S = 1$, it is possible to eliminate the unphysical states by introducing three-component fermions $\psi^T = (f_\uparrow f_0 f_\downarrow)$ with imaginary chemical potential $\lambda = -i\pi T/3$. The boundary conditions for Ψ on the imaginary part of the contour C_τ read as follows: $\Psi^\mu(\beta) = e^{i\pi/3}\Psi^\mu(0)$, $\bar{\Psi}^\mu(\beta) = e^{-i\pi/3}\bar{\Psi}^\mu(0)$. As a result, the distribution function in equilibrium is $f^{(1)}(\epsilon) = 1/[e^{\pm i\pi/3}\exp(\epsilon/T) + 1]$. Thus, the Schwinger-Keldysh formalism with 6×6 matrices for GF (6) and $f_\epsilon = f^{(1)}(\epsilon)$ in equilibrium is obtained. The off-diagonal Keldysh component is given by

$$G_0^K = -i2\pi\delta(\epsilon \pm h)$$
$$\times \left[B_1(\epsilon/T) \pm i\sqrt{3}\sinh\!\left(\frac{\epsilon}{2T}\right)\Big/\sinh\!\left(\frac{3\epsilon}{2T}\right)\right].$$

For arbitrary spin values $S > 1$ there is no unique imaginary chemical potential for $2S + 1$ component PF fermions, but instead they are distributed on each lattice site j according to

$$P(\lambda_j) = \sum_{l=0}^{[S-1/2]} a_l \delta(\lambda_j - \lambda_l),$$
$$a_l = \frac{2i}{2S + 1}\sin\!\left(\pi\,\frac{2l + 1}{2S + 1}\right),$$

where $\lambda_l = i\pi T(2l + 1)/(2S + 1)$ [13]. Thus, the Schwinger-Keldysh approach can be generalized for arbitrary spin values in the same fashion as for $S = 1/2$ and $S = 1$.

In summary, we derived the technique applicable for nonequilibrium dynamics of quantum spin systems. Un-

like other techniques this approach takes into account the constraint rigorously and allows one to treat spins on the same footing as Fermi and Bose systems. The method derived can be applied especially to problems where the local constraint becomes important, e.g., quantum phase transition in clean and disordered magnets, spin glasses, Kondo lattices, nonequilibrium Kondo systems, etc.

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